

Anomalous discrete chiral symmetry in the Gross-Neveu model and loop gas simulations

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Abstract

We investigate the discrete chiral transformation of a Majorana fermion on a torus. Depending on the boundary conditions the integration measure can change sign. Taking this anomalous behavior into account we define a chiral order parameter as a ratio of partition functions with differing boundary conditions. Then the lattice realization of the Gross-Neveu model with Wilson fermions is simulated using the recent ‘worm’ technique on the loop gas or all-order hopping representation of the fermions. An algorithm is formulated that includes the Gross-Neveu interaction for N fermion species. The critical line $m_c(g)$ is constructed for a range of couplings at $N = 6$ and for $N = 2$, the Thirring model, as examples.

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1 Introduction

Many textbooks on quantum field theory start with scalar fields and discuss, after preparing the arena with non-interacting free fields, the quartic self-coupling as the simplest conceivable interaction. At this stage renormalization or, on the lattice, the continuum limit has to be discussed in a non-trivial way. A mild generalization leads to N real scalar fields self-coupled by a unique quartic $O(N)$ invariant term. As is well known the kinetic term dictates the field dimension and implies a mass dimension $4 - D$ for the coupling constant. Thus the self-coupled scalar theory is renormalizable in $D = 4$. In fact, $D = N = 4$ is the standard model in the limit where all fields except the Higgs are stripped away. The perturbative renormalization group β -function is positive for small coupling and the models are hence perturbatively trivial. Simulations with simple lattice discretizations suggest that this features is also true nonperturbatively.

An analogous fermionic model can be written in terms of N ‘real’ Majorana fermions. Now, because there is only one derivative in the fermionic kinetic term, a quartic coupling has dimension $2 - D$. The renormalizable theory in $D = 2$ has in fact again a unique $O(N)$ invariant interaction. It has been proposed and considered in the limit of $N \rightarrow \infty$ a long time ago [1] and is now known as the Gross-Neveu (GN) model. For the sign of the quartic interaction that has been discussed to be the physically meaningful one in [1] the GN model is even asymptotically free. This feature that is shared by QCD was one of the main reasons for Gross and Neveu to study the model as an analog toy-model. The analogy goes even further as there also is a chiral symmetry in the GN model. Although it is only discrete, this symmetry involves the two-dimensional analog of γ_5 and is only present for massless fermions, which are thus distinguished by an enhanced symmetry. Gross and Neveu have shown that the chiral symmetry breaks spontaneously (at infinite N) and that mass generation and ‘dimensional transmutation’ take place. This beautiful parameter-free theory is then an analog of QCD in the chiral limit.

There have been some early efforts [2] to study this model beyond perturbation theory by Monte Carlo simulation. Attempts employing today’s standard techniques used for QCD [3] were made in [4] and [5]. However in [6] and [7] we have proposed techniques to simulate the fermionic Grassmann integral in a more direct and efficient way using its loop gas representation [8], see also [9] for a related effort. In this formulation, using Wilson fermions, the simulations resemble those for simple spin models with efficient algorithms. No nearly singular inversions and no nonlocal effective bosonic actions occur. While in more than two dimensions a sign problem still prevents the application of this technique [7] it is well suited for the GN model as we demonstrate below.

Like in QCD, the important chiral symmetry is violated by the Wilson dis-

cretization and an additive mass renormalization, i.e. a nontrivial definition of the critical point, is required. In this article we discuss, that, depending on the boundary conditions on a finite torus, an extra minus sign from the non-invariance of the Majorana fermion measure has to be taken into account in symmetry relations. We consider this as (a primitive form of) an anomaly. One such symmetry relation allows us to define a finite volume chiral order parameter. This way of defining the chiral point in parameter space is particularly convenient in the loop gas representation, where it corresponds to a well measurable topological variable.

After a definition of the model in section 2 the anomaly is discussed for the continuum theory in section 3 and connected with the fluctuating boundary conditions in section 4. In section 5 the loop gas representation and simulation on the lattice are described and numerical results are reported in section 6. Finally we end in section 7 with conclusions and an outlook.

2 $O(N)$ invariant Gross Neveu model

The $O(N)$ invariant GN model [1] is best written in terms of N self-coupled Majorana fermions $\xi_{\alpha,a}(x)$ with the Euclidean action

$$S = \int d^2x \frac{1}{2} \bar{\xi} (\gamma_\mu \partial_\mu + m) \xi - \frac{g^2}{8} (\bar{\xi} \xi)^2, \quad (1)$$

where the contracted index $a = 1, \dots, N$ refers to the global ‘flavor’ symmetry and $\alpha = 1, 2$ is spin. For a Majorana fermion $\bar{\xi}$ is not independent but just an abbreviation for

$$\bar{\xi} = \xi^\top \mathcal{C} \quad (2)$$

with the 2-dimensional Dirac matrices γ_0, γ_1 and the charge conjugation matrix \mathcal{C} satisfying

$$\gamma_\mu^\top = -\mathcal{C} \gamma_\mu \mathcal{C}^{-1}, \quad \mathcal{C} = -\mathcal{C}^\top, \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \quad (\gamma_\mu)^\dagger = \gamma_\mu. \quad (3)$$

In two dimensions the model is renormalizable in the strict sense, no other four-fermion interaction is compatible with the global $O(N)$. Moreover, the models with $N \geq 3$ are perturbatively asymptotically free. The Thirring model $N = 2$ has no divergent coupling renormalization. At vanishing fermion mass $m = 0$, there is in addition a discrete chiral invariance

$$\xi \rightarrow \gamma_5 \xi, \quad \gamma_5 = i\gamma_0 \gamma_1, \quad [\Rightarrow \bar{\xi} \rightarrow -\bar{\xi} \gamma_5]. \quad (4)$$

A standard step in treating the GN model, both in the continuum and on the lattice, is to factorize the interaction into bilinears at the expense of introducing a

scalar $\sigma(x)$. Foreclosing for a moment the lattice version, where d^2x becomes the cell volume a^2 , we write in the Boltzmann factor at each x

$$e^{\frac{a^2 g^2}{8} (\bar{\xi} \xi)^2} = \int_{-\infty}^{\infty} \frac{a d\sigma}{\sqrt{2\pi}} e^{-\frac{a^2}{2} \sigma^2 - \frac{a^2}{2} g \sigma \bar{\xi} \xi}. \quad (5)$$

This may be formally proven by shifting σ , but perhaps more convincingly, we state that both sides agree as polynomials in the nilpotent Grassmann bilinear $[(\bar{\xi} \xi)^{(N+1)} = 0]$.

After the introduction of $\sigma(x)$ we are led to the fermionic partition function

$$Z(m + g\sigma; \varepsilon) = \int D_\varepsilon \xi e^{-\frac{1}{2} \int d^2x \bar{\xi} (\gamma_\mu \partial_\mu + m + g\sigma) \xi} = \text{Pf}[\mathcal{C}(\gamma_\mu \partial_\mu + m + g\sigma)] \quad (6)$$

as the basic fermionic building block. In this formula ξ represents only one flavor. We imagine this fermionic functional integral here formally on a finite torus of extent $L_0 \times L_1$ in the continuum. The two component ('bits') object ε with $\varepsilon_\mu \in \{0, 1\}$ labels four possible (anti)periodic boundary conditions

$$\xi(x \pm \hat{\mu} L_\mu) = (-1)^{\varepsilon_\mu} \xi(x). \quad (7)$$

The Pfaffian Pf is the counterpart of the determinant associated with Dirac fermions. Note that Pf is only defined for antisymmetric matrices and that the operator in (6) [absorbing m and g now into σ]

$$A(\sigma) = \mathcal{C}(\gamma_\mu \partial_\mu + \sigma) = -A^\top(\sigma) \quad (8)$$

indeed has this property for all four choices of ε . One relation for Pfaffians is that they square to determinants,

$$(\text{Pf}[A(\sigma)])^2 = \text{Det}[A(\sigma)]. \quad (9)$$

Note that the sign of Pf, which is our focus in the next section, is not determined by the determinant.

3 Symmetry of the Pfaffian in a finite volume

By a suitable choice of Dirac matrices A can be taken to be real. Hence its eigenvalues are imaginary and come in pairs

$$A(\sigma)f = i\lambda f, \quad A(\sigma)f^* = -i\lambda f^*. \quad (10)$$

In addition, by using γ_5 , it is trivial to demonstrate that $A(-\sigma)$ possesses precisely the *same pairs* of eigenvalues. By arguments analogous to those used for Weyl

fermions¹ in connection with the global anomaly [10] a functional definition of the Pfaffian as a root of the determinant has to be smooth under deformations of σ . For some reference field σ where there are no vanishing eigenvalues we define the Pfaffian by multiplying all positive eigenvalues λ only. This represents a certain definition of the (irrelevant) over-all phase. A possible simple reference field would be $\sigma(x) \equiv m > 0$, the free massive Majorana fermion. Then the Pfaffian for other field configurations including its sign follows from smoothness.

Again as in [10] this requires us to follow the flow of individual eigenvalues as functionals of σ . As a pair of them crosses zero the associated eigenvectors allow us to follow the members of the pair separately and defines a unique continuation of the phase of the Pfaffian through the crossing. From the spectral properties discussed above we conclude that $Z[\sigma; \varepsilon]$ must be either symmetric or antisymmetric in σ

$$Z(\sigma; \varepsilon) = \pi(\varepsilon)Z(-\sigma; \varepsilon), \quad \pi(\varepsilon) \in \{+1, -1\}. \quad (11)$$

In the next paragraph we shall show that

$$\pi(\varepsilon) = \begin{cases} -1 & \text{for } \varepsilon_\mu = (0, 0) \\ +1 & \text{for } \varepsilon_\mu = (1, 0), (0, 1), (1, 1) \end{cases} \quad (12)$$

holds.

We consider an interpolation

$$g(t) = Z(t\sigma; \varepsilon) = \text{Pf}[A(t\sigma)], \quad t \in [-1, 1] \quad (13)$$

and assume $Z[\sigma; \varepsilon] \neq 0$ as otherwise the proof is trivial. Then the question of (anti)symmetry in t can be ‘decided’ in an infinitesimal neighborhood of $t = 0$ which we can control by leading order perturbation theory.

Except for $\varepsilon_\mu = (0, 0)$ the eigenvalues at $t = 0$ do not vanish but are of order L_μ^{-1} . Hence there is no zero-crossing, which proves the lower line of (12). In the totally periodic case there is a pair of x -independent zero-modes. The 2-spinors u_\pm are chosen to diagonalize the spin matrix of the perturbation $\mathcal{C}t\sigma$

$$\mathcal{C}u_\pm = \pm iu_\pm, \quad A(0)u_\pm = 0. \quad (14)$$

Now in leading order degenerate perturbation theory we find two eigenvalues

$$\lambda_\pm \simeq \pm \frac{t}{L_0 L_1} \int d^2 x \sigma(x) \quad (15)$$

associated with these eigenvectors.

¹We admit here that our arguments about infinite objects disregarding renormalization are at a highly formal level. However, this will be substantiated on the lattice in our case.

Unless this integral vanishes we see that exactly one pair of eigenvalues crosses zero as we move $t = 0 + \epsilon \rightarrow t = 0 - \epsilon$ and hence the Pfaffian changes sign. The sign π cannot jump with σ . Thus, if the integral above vanishes, i.e. σ has a vanishing zero-momentum component, we deform σ a little such that this is not the case anymore. Now (12) is established.

We note that our general result above is consistent with the explicit evaluation in the continuum limit of the Wilson-Pfaffian for constant σ , see appendix A in [6]. Inspired by this calculation we give another formal proof of the above result for a continuum theory regularized by a cut-off in momentum space. We start from the identities

$$\gamma_5^\top A(\sigma) \gamma_5 = A(-\sigma) \quad (16)$$

and

$$\text{Pf}[\gamma_5^\top A(\sigma) \gamma_5] = \text{Det } \gamma_5 \text{Pf}[A(\sigma)]. \quad (17)$$

The Det in the last line is taken in the function space over which $\xi_\alpha(x)$ is integrated (with anticommuting expansion coefficients). If Pf is written as a Grassmann integral, then $\text{Det } \gamma_5$ is the Jacobian of $\xi \rightarrow \gamma_5 \xi$. Each 2×2 block contributes a factor $\det \gamma_5 = -1$ in the usual sense. We now imagine to regularize the fermion integral by a finite mode number cutoff. If we impose this cutoff in a way preserving the symmetry of rotations by π then for each incorporated mode p_μ also $-p_\mu$ has to be included. This leads to an odd total mode number only for $\varepsilon_\mu = (0, 0)$ because of the unpaired mode $p_\mu = (0, 0)$. Thus we have

$$\text{Det } \gamma_5 = \pi(\varepsilon) \quad (18)$$

representing a non-invariance of the integration measure in the case of fully periodic boundary conditions. It also follows from the foregoing discussion that expectation values in the GN model at odd N with such boundary conditions are ill defined at the chiral point in any finite volume, because the normalizing partition function vanishes. This arises at least superficially in a similar fashion as with the global anomaly in [10].

4 Observables from fluctuating boundary conditions

4.1 Chiral order parameter

We have introduced four different boundary conditions for the fermions in the GN model. We may consider the choice among them as an additional dynamical

variable and consider general superpositions with an amplitude $z(\varepsilon)$

$$\tilde{Z}(\sigma; z) = \sum_{\varepsilon} z(\varepsilon) Z(\sigma; \varepsilon). \quad (19)$$

Below we shall be interested in two special choices for the amplitudes

$$z_+(\varepsilon) = \frac{1}{2} - \delta_{\varepsilon, (0,0)}, \quad z_-(\varepsilon) = \frac{1}{2}. \quad (20)$$

The first choice is distinguished by leading to a strictly positive hopping or world-line expansion for the finite volume GN model on the lattice [6]. The anomalous symmetry (including the sign of $\text{Det}\gamma_5$) found in the previous section implies the relation

$$\tilde{Z}(-\sigma; z_+) = \tilde{Z}(\sigma; z_-). \quad (21)$$

For either choice — jointly for all flavors — we find partition functions for the interacting GN model

$$Z_{\pm}^{\text{GN}}(m, g) = \int D\sigma e^{-\frac{1}{2} \int d^2x \sigma^2} [\tilde{Z}(m + g\sigma; z_{\pm})]^N \quad (22)$$

which coincide at the chiral point $m = 0$ as one shows by transforming $\sigma \leftrightarrow -\sigma$. We hence may define an order parameter that vanishes at the chiral point

$$\chi = \frac{1}{N} \ln(Z_-^{\text{GN}}/Z_+^{\text{GN}}). \quad (23)$$

More conventional order parameters may be based on chirally odd observables $\bar{\xi}(x)\xi(y)$. In view of our later simulations we define

$$\begin{aligned} \langle \xi_{\alpha a}(u) \bar{\xi}_{\beta b}(v) \rangle_z &= \frac{\delta_{ab}}{Z_+^{\text{GN}}} \int D\sigma e^{-\frac{1}{2} \int d^2x \sigma^2} [\tilde{Z}(m + g\sigma; z)]^{N-1} \\ &\times \sum_{\varepsilon} z(\varepsilon) \int D_{\varepsilon} \xi e^{-\frac{1}{2} \int d^2x \bar{\xi}(\gamma_{\mu} \partial_{\mu} + m + g\sigma) \xi} \xi_{\alpha}(u) \bar{\xi}_{\beta}(v). \end{aligned} \quad (24)$$

Here we indicated the periodicity in the integration measure. Note that we always normalize with respect to the z_+ ensemble. Such correlations are $2L_{\mu}$ -periodic but neither periodic nor antiperiodic over the original torus while bilinear local densities remain periodic. Chiral symmetry implies

$$\gamma_5 \langle \xi_{\alpha a}(u) \bar{\xi}_{\beta b}(v) \rangle_{z_{\pm}} \gamma_5 = -\langle \xi_{\alpha a}(u) \bar{\xi}_{\beta b}(v) \rangle_{z_{\mp}}. \quad (25)$$

An integration over a $2L_1$ long interval projects to the spatially periodic component at zero spatial momentum and we obtain the chirally odd scalar k_S

$$k_S(x_0) = -\frac{1}{2N} \int_{-L_1}^{+L_1} dx_1 [\langle \bar{\xi}(0) \xi(x) \rangle_{z_+} + \langle \bar{\xi}(0) \xi(x) \rangle_{z_-}] \quad (26)$$

with both ξ indices contracted here. For the purpose of monitoring the field normalization we define in addition

$$k_V(x_0) = -\frac{1}{N} \int_{-L_1}^{+L_1} dx_1 \langle \bar{\xi}(0) \gamma_0 \xi(x) \rangle_{z_+}. \quad (27)$$

We only use z_+ boundary conditions here, as they will lead to the highest precision on the lattice. In this way k_V has both chirally even and odd components. Due to parity, k_S is an even function of x_0 while k_V is odd.

We form the ratio k_S/k_V to cancel multiplicative renormalization factors. While with exact chiral symmetry k_S vanishes, with a regularization that violates chiral symmetry by effects linear in the lattice spacing a we can only expect to find $k_S(x_0) = O(a)$ if $\chi = 0$ has been imposed as a renormalization condition. We therefore tie x_0 to a physical length scale to obtain a scaling situation and define

$$\tilde{\chi}_n = \frac{k_S(nL_0/4)}{k_V(L_0/2)} \quad (n = 1, 2, 3) \quad (28)$$

as universal quantities vanishing in the continuum limit at the chiral point. The finite size L_0 supplies an infrared regulator and keeps our model well-defined (for the boundary conditions chosen) at the chiral point in a finite volume. This is similar to the Schrödinger functional of QCD [11], where the PCAC relation replaces the discrete chiral symmetry relations invoked here.

5 Lattice, Wilson fermions, loop gas

To pass to the lattice formulation we restrict $\xi(x)$ to the sites of a toroidal square lattice with spacing a and integer (anti)periodicity lengths L_μ/a . In addition we replace the Dirac operator in (6) and (8) by the Wilson matrix (with $r = 1$)

$$\gamma_\mu \partial_\mu \rightarrow \gamma_\mu \tilde{\partial}_\mu - \frac{a}{2} \partial_\mu \partial_\mu^*. \quad (29)$$

We use here standard notation and $\partial_\mu, \partial_\mu^*, \tilde{\partial}_\mu$ denote the forward, backward and symmetrized nearest neighbor difference operators. The second term eliminates the doubler modes but also breaks the chiral symmetry (4) just like a mass term. The consequences of chiral symmetry however are expected to emerge in the continuum limit. To reach it one has to determine a critical value $m_c(g)$ as there is no symmetry to prevent an additive mass renormalization. From here on we use lattice units and set $a = 1$.

5.1 Loop gas representation of the GN model

The Wilson-discretized GN model has already been studied in [4], [5] by hybrid Monte Carlo methods and Majorana-Wilson fermions were simulated in [6] by a cluster algorithm in the loop gas representation elaborating on [8]. Most recently we have studied a worm algorithm [7] and we will now make extended use of results from this paper which should be consulted for details.

In [6] we have shown that the Grassmann integral (24) — for one flavor at this point — can be written as a sum over contributions from non-intersecting loops on the lattice with one additional open string connecting the locations of the field insertions u and v . The underlying loop ensemble is

$$\mathcal{Z} = \sum_{u,v,\{k(l)\}} \Theta(k; u, v) 2^{-\bar{C}/2} \prod_{x \in \mathcal{M}[k]} (2 + m + g\sigma(x)). \quad (30)$$

In this formula the link variables $k(l) = 0, 1$ are one on the loops/string and zero elsewhere. We also say that links with $k(l) = 1$ carry dimers. The constraint $\Theta(k; u, v) = 0, 1$ restricts the k configurations to the subset corresponding to the hopping expansion of the Majorana Wilson fermion with field insertions at u, v . It demands that zero or two dimers are attached to all sites except u, v if they do not coincide. In this case they must see exactly one dimer each, the beginning and end of the string connecting them. The integer \bar{C} counts corners, sites connected to two orthogonal dimers. Finally the monomer set $\mathcal{M}[k]$ for each configuration k consists of all sites with no dimers attached.

For each k -configuration we define topological variables $e_\mu[k] \in \{0, 1\}$ as follows. For each direction μ on the torus we distinguish one sheet orthogonal to the μ -direction (a line for $D = 2$) of links in that direction. This is the same construction that is used in connection with the center symmetry in lattice gauge theory. A definite convention is given in [7]. Then e_μ is zero or one depending on whether an even or odd number of dimers belong to the sheet. Thus we decompose the loop gas into four classes, see [6]. If a contribution has $u = v$, $\theta(k, u, u) = 1$ there are only closed loops and e_μ coincides with their total mod 2 winding number in the respective direction. We also associate possible antiperiodic boundary conditions with minus signs on bonds in the respective sheets where we ‘close the torus’. Now the fermionic partition function is given by

$$\tilde{Z}(\sigma; z) = \sum_k \Theta(k; 0, 0) 2^{-\bar{C}/2} \prod_{x \in \mathcal{M}[k]} (2 + \sigma(x)) \Phi(e; z) \quad (31)$$

where we took $u = v = 0$ to only sum over closed loop ‘vacuum’ configurations. The amplitude Φ is

$$\Phi(e; z) = (2\delta_{e,(0,0)} - 1) \sum_\varepsilon z(\varepsilon) (-1)^{\varepsilon \cdot e}. \quad (32)$$

The first factor stems from spin and Fermi statistics in the Grassmann integral (see [6], [7]). In particular it is +1 for all topologically trivial loop configurations which amounts to the absence of a ‘hard’ sign problem in two dimensions. The second factor corresponds to the fluctuating boundary conditions. If we now insert $z = z_{\pm}$ from (20) we find

$$\Phi(e; z_+) = 1, \quad \Phi(e; z_-) = 2\delta_{e,(0,0)}, \quad (33)$$

and in particular the announced positivity for the z_+ ensemble.

To pass to the partition function of the interacting GN model we insert the loop representation simultaneously for all flavors and find

$$Z_{\pm}^{\text{GN}}(m, g) = \sum_{k_1 \dots k_N} \prod_{a=1}^N [\Theta(k_a; 0, 0) 2^{-\bar{C}_a/2} \Phi(e_a; z_{\pm})] \prod_x c(M(x)). \quad (34)$$

In this formula k_a, \bar{C}_a, e_a are defined as before, just for each flavor independently. The field $M(x)$ with possible values $0, 1, \dots, N$ depends on all k_a (left implicit) and yields the total number of monomers at x , i.e. it counts to how many $\mathcal{M}[k_a]$ the site x belongs. The various flavors thus interact through the factor

$$c(M) = \int_{-\infty}^{\infty} \frac{d\sigma}{\sqrt{2\pi}} e^{-\frac{1}{2}\sigma^2} [2 + m + g\sigma]^M. \quad (35)$$

The weights $c(M)$ may conveniently be generated from a recursion formula. In the Monte Carlo updates below we shall rather need ratios

$$r(M) = \frac{c(M+1)}{c(M)} \quad (36)$$

which are directly generated by

$$r(0) = 2 + m, \quad r(M) = 2 + m + \frac{g^2 M}{r(M-1)}. \quad (37)$$

5.2 GN worm algorithm

Finally in our simulation we sample the ensemble

$$\mathcal{Z}^{\text{GN}} = \sum_{j, u, v, \{k_a\}} \Theta(k_j; u, v) 2^{-\bar{C}_j/2} \prod_{a \neq j} [\Theta(k_a; 0, 0) 2^{-\bar{C}_a/2}] \prod_x c(M(x)). \quad (38)$$

The summation now includes a sum over $j = 1, 2, \dots, N$ which is an ‘active’ flavor to which the insertions u, v refer. A valid update procedure is given by simply

using the algorithm of [7] for the active flavor with the external field replaced $c(M(x))$ which depends also on the non-active flavors that are momentarily frozen during the update. Whenever $u = v$ is encountered the active flavor is changed randomly and ergodicity is achieved. We summarize the whole procedure in the following paragraph.

The simulation alternates between analogous u -updates and v -updates, of which we only detail the latter. In addition we alternate between type I and II. Type I involves:

- Pick a nearest neighbor v' of v , call the link $l = \langle vv' \rangle$
- Propose the combined move $v \rightarrow v'$, $k_j(l) \rightarrow 1 - k_j(l)$
- Compute the ratio q of the weight given in [7] after and before the move where we suitably substitute $r(M)$ for the external field ratio. The Metropolis decision is controlled by $|q|$.

In step II one only acts if $u = v$ is met. In this case we:

- Pick a random new value $j \in \{1, 2, \dots, N\}$ for the active flavor. We may actually imagine this as a Metropolis proposal tried after every type I move. Whenever $u \neq v$ holds it will be rejected due to the θ -constraints while for $u = v$ it is accepted with probability one.
- With probability p_{kick} we re-locate $u = v$ randomly on the lattice.

5.3 Observables in the loop gas representation

We define expectation values in the ensemble (38)

$$\langle\langle \mathcal{O} \rangle\rangle = \frac{1}{\mathcal{Z}^{\text{GN}}} \sum_{j,u,v,\{k_a\}} \mathcal{O} \Theta(k_j; u, v) 2^{-\bar{C}_j/2} \prod_{a \neq j} [\Theta(k_a; 0, 0) 2^{-\bar{C}_a/2}] \prod_x c(M(x)) \quad (39)$$

where \mathcal{O} may depend on all quantities that are summed over. The chiral order parameter χ (23) is easily measured by

$$e^{N\chi} = \frac{\langle\langle \prod_a \Phi(e_a; z_-) \delta_{u,v} \rangle\rangle}{\langle\langle \delta_{u,v} \rangle\rangle} = \frac{\langle\langle \prod_a [2\delta_{e_a, (0,0)}] \delta_{u,v} \rangle\rangle}{\langle\langle \delta_{u,v} \rangle\rangle}. \quad (40)$$

In other words, at the chiral point $\chi = 0$ the fraction 2^{-N} of all vacuum ($u = v$) configurations has the trivial topology in all flavours simultaneously. In the trivial case $g = 0$ this arises for $m = 0$ from independent factors $1/2$ for each species.

Other observables considered in this paper are the correlations

$$\langle \xi_a(x) \bar{\xi}_b(0) \rangle_z = \delta_{ab} \frac{\langle \langle \sum_{\varepsilon} z(\varepsilon) (-1)^{\varepsilon \cdot e_j} \delta_{x,u-v}^{(\varepsilon)} \psi_j \mathcal{S}(k_j; u, v) \prod_{c \neq j} \Phi(e_c; z) \rangle \rangle}{\langle \langle \delta_{u,v} \rangle \rangle}. \quad (41)$$

Here $\delta^{(\varepsilon)}$ is the ε -(anti)periodic lattice δ function and the spin matrix² \mathcal{S} has been defined in [7]. It carries two spin indices that we suppressed at $\xi, \bar{\xi}$. The sign ψ_j collects the phases from spin matrix elements and fermion loops in the active flavor, see eq. (48) in [7]. It is evolved during the updates and thus available at every step. Applying this correspondence for k_S and k_V in (26), (27), using (33), we arrive at the translations

$$k_V(x_0) = \frac{\langle \langle \psi_j \text{tr}[\gamma_0 \mathcal{S}(k_j; u, v)] [(-1)^{e_{0,j}} \delta_{x_0, u_0 - v_0}^{(1)} - \delta_{x_0, u_0 - v_0}^{(0)}] \rangle \rangle}{\langle \langle \delta_{u,v} \rangle \rangle} \quad (42)$$

and

$$k_S(x_0) = \frac{\langle \langle \psi_j \text{tr}[\mathcal{S}(k_j; u, v)] [(-1)^{e_{0,j}} \delta_{x_0, u_0 - v_0}^{(1)} E_j^+ - \delta_{x_0, u_0 - v_0}^{(0)} E_j^-] \rangle \rangle}{\langle \langle \delta_{u,v} \rangle \rangle} \quad (43)$$

with

$$E_j^{\pm} = \frac{1}{2} \left(1 \pm \prod_{a \neq j} [2\delta_{e_a, (0,0)}] \right). \quad (44)$$

At $x_0 = L_0/2$, due to parity covariance, $\delta^{(0)}$ in k_V and $\delta^{(1)}$ in k_S do not contribute. Although these expressions may look somewhat intimidating, all quantities entering are readily available from the updates and the accumulation proceeds quickly in the form of histograms with bins for each time separation $u_0 - v_0$ and each of the four possible e_j . To debug the code we have found it useful to run at $g = 0$ comparing with the known exact answers.

6 Numerical tests in the Gross-Neveu model

We have generalized the code described in [7] to include an arbitrary number of flavors coupled by the interaction term (35) and we thus sample the ensemble (38). We have accumulated the necessary observables entering into χ and $\tilde{\chi}_n$, $n = 1, 2, 3$. By consulting perturbation theory and some preliminary experiments, we have run series of simulations varying L at fixed bare coupling g with a value m such that $\chi = 0$ holds up to a few sigma deviation. This is facilitated by the fact that m_c seems to hardly vary with L at fixed g . For each of the observables considered,

²The case $u = v$ is special in the definition of \mathcal{S} . It would depend on $M(u)$ here but will not be required as we will not consider correlations with coinciding arguments ($x = 0$).

for example those in (40), we also compute its derivative with respect to m . This is achieved by introducing another observable W_m , the derivative of the logarithm of the Boltzmann weight with respect to m ,

$$\frac{\partial}{\partial m} \prod_x c(M(x)) = W_m \prod_x c(M(x)), \quad W_m = \sum_x \frac{M(x)}{r(M(x)-1)}, \quad (45)$$

which is also easy to keep track of during the simulations. Now m -derivatives of not explicitly m -dependent observables \mathcal{O} are given by connected correlations

$$\frac{\partial}{\partial m} \langle \langle \mathcal{O} \rangle \rangle = \langle \langle \mathcal{O} W_m \rangle \rangle - \langle \langle \mathcal{O} \rangle \rangle \langle \langle W_m \rangle \rangle. \quad (46)$$

Thus we obtain estimates for $\partial\chi/\partial m$ and, forming quotients, also $\partial\tilde{\chi}_n/\partial\chi$ (considering g fixed). All these quantities are functions of primary expectation values and they are estimated including errors by the technique presented in [12]. By exploiting the derivatives we can effectively ‘post-run’ vary m a little bit to solve the tuning problem of finding the value m_c where χ vanishes. This is equivalent to reweighting in m with a first order Taylor expansion of the Boltzmann factor. We thus for example obtain an estimate for $m_c = m + \delta m$ with

$$\delta m = -\chi \frac{1}{\partial\chi/\partial m} = m - \frac{\langle \langle \mathcal{O} \delta_{u,v} \rangle \rangle \langle \langle \delta_{u,v} \rangle \rangle \ln[\langle \langle \mathcal{O} \delta_{u,v} \rangle \rangle / \langle \langle \delta_{u,v} \rangle \rangle]}{\langle \langle \mathcal{O} W_m \delta_{u,v} \rangle \rangle \langle \langle \delta_{u,v} \rangle \rangle - \langle \langle \mathcal{O} \delta_{u,v} \rangle \rangle \langle \langle W_m \delta_{u,v} \rangle \rangle} \quad (47)$$

with

$$\mathcal{O} = \prod_a [2\delta_{e_a, (0,0)}] \quad (48)$$

in this case. Since χ is expected to be a smooth function of mL we expect that derivatives with respect to mL are order one. Then, for small χ the next Taylor term can be roughly expected to be $O(\chi\delta m)$ which we monitor to be negligible compared to the statistical error of δm and hence m_c . Where this not true, the initial tuning of m was not good enough for first-order reweighting and the run has to be repeated closer to the chiral point. The range of possible corrections gets smaller as the number of lattice sites grows because of the variance of the estimate of the derivative.

The entries in table 1 have been constructed in this way. Similarly as in the above discussion we have estimated the combination $\tilde{\chi}_n - (\partial\tilde{\chi}_n/\partial\chi)\chi$ to correct for tiny nonzero χ . Often this systematic correction is insignificant, within one standard deviation, but the variance and thus the error is reduced due to anticorrelated fluctuations of the terms. Each line in table 1 is based on a run of 8×10^7 iterations, where an iteration performs L^2 elementary moves (counting u and v).

The first series is at $g^2 = 1, N = 2$ in the Thirring model. We expect no divergent coupling renormalization in this case and a continuum limit could be

N	g^2	m	L	m_c	$\tilde{\chi}_1$	$\tilde{\chi}_2$	$\tilde{\chi}_3$
2	1	-0.4626	8	-0.46249(22)	-0.0387(5)	-0.0252(4)	-0.0132(5)
2	1	-0.4626	16	-0.46236(15)	-0.0198(8)	-0.0134(6)	-0.0068(8)
2	1	-0.4626	32	-0.46254(13)	-0.0092(14)	-0.0074(9)	-0.0049(13)
2	1	-0.4626	64	-0.46275(14)	-0.0037(30)	-0.0030(20)	-0.0052(30)
6	0.3	-0.5967	8	-0.59622(35)	-0.0379(19)	-0.0303(18)	-0.0236(17)
6	0.3	-0.5967	16	-0.59634(22)	-0.0263(27)	-0.0169(27)	-0.0116(26)
6	0.3	-0.5967	32	-0.59693(16)	-0.0182(44)	-0.0093(42)	-0.0099(40)
6	0.3	-0.5967	64	-0.59663(26)	-0.015(25)	-0.011(17)	-0.012(11)
6	0.4	-0.8007	8	-0.80075(36)	-0.0558(19)	-0.0389(18)	-0.0286(17)
6	0.4	-0.8007	16	-0.80060(21)	-0.0312(29)	-0.0200(28)	-0.0121(26)
6	0.4	-0.8007	32	-0.80077(15)	-0.0246(47)	-0.0119(45)	-0.0014(42)
6	0.4	-0.8007	64	-0.80081(17)	-0.016(19)	-0.015(14)	-0.016(10)
6	0.5	-1.0058	8	-1.00516(36)	-0.0707(19)	-0.0423(18)	-0.0256(18)
6	0.5	-1.0058	16	-1.00567(21)	-0.0471(31)	-0.0202(29)	-0.0071(28)
6	0.5	-1.0058	32	-1.00601(16)	-0.0250(56)	-0.0038(52)	0.0066(50)
6	0.5	-1.0063	64	-1.00612(33)	0.059(69)	0.050(37)	0.025(20)

Table 1: Simulation results for m_c defined by $\chi = 0$ and variant chiral order parameters $\tilde{\chi}_n = O(a)$ at $m = m_c$.

reached at fixed bare g , but the linearly divergent mass renormalization of Wilson fermions is present. As an asymptotically free example, data were taken for $N = 6$. We notice in the table that the L dependence of m_c is very weak. A systematic trend is barely visible. In figure 1 we plot our results for m_c (taken from $L = 64$) for $N = 6$, with the dominant one loop contribution subtracted, against g^4 . The dotted line corresponds to the curve

$$m_c \approx \sum_{n=1}^3 \bar{m}_c^{(n)} g^{2n}, \quad \bar{m}_c^{(1)} = m_c^{(1)} \quad \bar{m}_c^{(2)} = -0.270, \quad \bar{m}_c^{(3)} = 0.189, \quad (49)$$

where $m_c^{(1)}$ is the perturbative result (66) (see appendix A).

It perfectly represents our data at the given error-level, but $\bar{m}_c^{(i)}$ need not coincide with the true perturbative coefficients $m_c^{(i)}$, $i = 2, 3$ that are not known to us.

For $N = 2$ the only physical scale is L and we expect $\tilde{\chi}_n$ to vanish proportional to a/L as chiral symmetry emerges in the continuum limit. A glance at the table shows that this is true within errors. For $N \geq 3$ asymptotic freedom holds and the situation is different. The continuum limit is expected to occur for $g^2 \searrow 0$. At least at large N [1] we know that the physics is governed by an effective potential which for any g^2 has a critical L_c such that there is one minimum for $L < L_c$ but

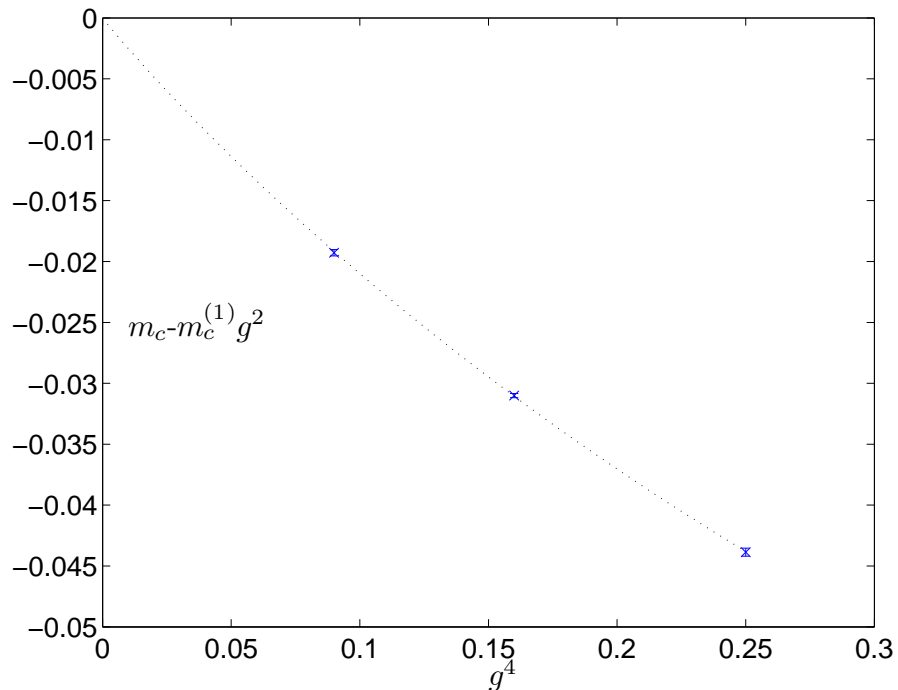


Figure 1: Values of the critical mass m_c in lattice units at $N = 6$ after the subtraction of the 1-loop contribution.

two minima for larger $L > L_c$ [13]. At $L = \infty$ a fermion mass m_R is generated spontaneously and emerges as a nonperturbative scale, somewhat analogous to Λ_{QCD} . Therefore we expect for our $N = 6$ series a scaling behavior

$$\tilde{\chi}_n = \frac{a}{L} f_n(m_R L) \quad (50)$$

with nontrivial but presumably smooth functions f_n .

At small g we expect $m_R L$ to be tiny for $L \leq 64$ appearing in the table and we may replace the scaling function by $f_n(m_R L) \approx f_n(0)$ and thus the situation is similar to the Thirring model. This is still roughly so for the couplings $g^2 \leq 0.5$ studied here. An investigation of the GN model at large N on the lattice with Wilson fermions has suggested that for $N = 6, g^2 = 0.5$ the value L_c may be not far from our L values, with quite some uncertainty however at finite N . On the other hand the results in [13] suggest $m_R L_c = \mathcal{O}(1)$ and we may be close to the onset of a change in the scaling behavior.

In our data analysis we obtain information on autocorrelation times $\tau_{\text{int}, \mathcal{O}}$ for all primary and derived observables that we study. To avoid too much data handling we stored sub-histograms from 800 successive iterations resulting in a length of 10^5

of our time series. Between these blocked measurements autocorrelation times were small but sometimes still measurable. Under these conditions our error estimates are accurate at the percent level for the error of the error [12]. To obtain more detailed dynamical information we made some shorter runs of 10^6 blocks of only $N = 6$ iterations each. This has yielded $\tau_{\text{int},\chi} = 2.06(6), 3.47(14), 9.3(6), 69(10)$ for $g^2 = 0.4$ and $L = 8, 16, 32, 64$. The unit of τ_{int} is now ‘steps per site and flavor’. We see critical slowing down here, especially for the step $32 \rightarrow 64$. This may be related to approaching a physically ‘difficult’ volume. The simulations of free fermions in [7] have shown very little slowing down. The less favorable, but still not too bad, performance here is probably related to the flavors holding back each other. With growing coupling the different flavors get more more correlated, but they are only updated ‘one at a time’ with the others frozen until $u = v$ is met. One could in principle try to influence the frequency of this by introducing a weight $\rho(u - v)$ as done in [14] for the Ising model. In addition a second active flavor, needed anyway to simulate four-point functions, could be beneficial here.

7 Conclusions and outlook

We have successfully incorporated the GN interaction in the loop gas representation of Majorana fermions and found the algorithm of [7] to remain rather efficient although some critical slowing down is visible. We have clarified the anomalous discrete chiral symmetry behavior in a finite volume. It can be used to define the chiral continuum limit with Wilson fermions by monitoring a topological observable χ related to fluctuating boundary conditions in the finite volume loop gas. It serves a purpose similar to the PCAC relation in the Schrödinger functional scheme for QCD and makes the required mass fine-tuning quite manageable. To complete the definition of a finite volume scheme for the GN model we at present still lack a good definition of a running coupling in a finite volume. The quantity proposed in [4] will presumably be a good choice but it requires the extension of the algorithm to also sample four-point functions. This seems feasible and will be required in any case to be able to probe mass ratios for which exact conjectures have been made [15]. It also seems advisable to implement on-shell Symanzik $O(a)$ improvement as in QCD. The action has to be augmented by only one term, $(\bar{\xi}\xi)^3$ for example, but in addition the elementary fermion operator ξ needs to be improved as it can mix with $\xi(\bar{\xi}\xi)$. It would presumably be a good idea, interesting in itself, to first test this at large N on the lattice with an analytic but nonperturbative calculation. In the end it may hopefully also be possible to shed some light on the special cases $N = 3, 4$ which may be supersymmetric models in disguise [16].

From the algorithmic point of view we have seen here that with the sign problem absent in two dimensions (apart from a milder form in the finite size effects) we

could simulate a physically interesting interacting fermionic theory with the all-order strong coupling/hopping reformulation as an alternative to HMC methods [3].

A Some perturbative results

In this appendix we explore in lattice perturbation theory to order g^2 some of the quantities that were studied numerically before. To evaluate quantities in leading order perturbation theory, it is useful to exploit the fact that the Grassmann integrals for each individual flavor are linear in each $\sigma(x)$ because it multiplies the bilinear $\bar{\xi}\xi$ at x whose square vanishes. Hence one derives

$$\frac{\partial}{\partial\sigma(x)}\tilde{Z}(\sigma; z) = \tilde{Z}(\sigma; z)\tilde{K}(\sigma; z), \quad \frac{\partial^2}{\partial\sigma(x)^2}\tilde{Z}(\sigma; z) = 0 \quad (51)$$

with

$$\tilde{K}(\sigma; z) = \frac{1}{2}\text{tr}\tilde{G}(0; \sigma; z) \quad (52)$$

and

$$\tilde{G}(x; \sigma; z) = \frac{\sum_{\varepsilon} z(\varepsilon) Z(\sigma; \varepsilon) G(x; \sigma; \varepsilon)}{\tilde{Z}(\sigma; z)} \quad (53)$$

which is given in terms of propagators $G(x; \sigma; \varepsilon)$ inverse to $\gamma_{\mu}\tilde{\partial}_{\mu} - \frac{1}{2}\partial_{\mu}\partial_{\mu}^{*} + \sigma$ with fixed boundary conditions ε . Due to translation invariance we find

$$\frac{\partial}{\partial\sigma(x)}\tilde{Z}(m + g\sigma; z)|_{g=0} = \frac{g}{V}\frac{\partial}{\partial m}\tilde{Z}(m; z) \quad (54)$$

with the volume $V = L_0L_1$, and similarly

$$\sum_x \frac{\partial}{\partial\sigma(x)}\tilde{Z}(m + g\sigma; z)\tilde{G}(x; m + g\sigma; z)|_{g=0} = g\frac{\partial}{\partial m}\tilde{Z}(m; z)\tilde{G}(x; m; z). \quad (55)$$

In addition we can make use of

$$\frac{\partial^2}{\partial\sigma(x)^2}\tilde{Z}(\sigma; z)\tilde{G}(x; \sigma; z) = 0. \quad (56)$$

There is a small subtlety here. The vanishing of the doubly periodic partition function $Z(0, (0, 0)) = 0$ trivially implies $\tilde{Z}(0; z_+) = \tilde{Z}(0; z_-)$. A singularity in the propagator $G(x; m; (0, 0)) \simeq (mL_0L_1)^{-1} + O(m^0)$ lifts however the zero-mode and yields an $O(a)$ difference

$$\lim_{m \rightarrow 0} [\tilde{K}(m; z_-) - \tilde{K}(m; z_+)] = \frac{2c_{00}}{\sqrt{(L_0^2 + L_1^2)/2}}. \quad (57)$$

The constant derives from sums over momenta appropriate for the respective boundary conditions and the numerical Symanzik expansion (see appendix D of [17]) yields

$$c_{00} = \frac{\lim_{m \rightarrow 0} Z(m; (0, 0)) / (mL)}{\sum_{\varepsilon \neq (0, 0)} Z(0; \varepsilon)} = 0.155609865 - \frac{0.20668}{L^2} + O(L^{-4}). \quad (58)$$

Here and below we perform the numerical evaluations for $L_0 = L_1 = L$. If we write $\tilde{K}(0; z_-) - \tilde{K}(0; z_+)$ below we refer to (57).

A.1 Chiral order parameter χ

With the help of the above formulas it is now rather easy to derive

$$Z_{\pm}^{\text{GN}}(m, g) = [\tilde{Z}(m; z_{\pm})]^N \left\{ 1 + \frac{g^2}{2} N(N-1) V \tilde{K}(m; z_{\pm})^2 \right\} + O(g^4) \quad (59)$$

and hence

$$\chi = \ln[\tilde{Z}(m; z_-) / \tilde{Z}(m; z_+)] + \frac{g^2}{2} (N-1) V [\tilde{K}(m; z_-)^2 - \tilde{K}(m; z_+)^2] + O(g^4) \quad (60)$$

The perturbative Ansatz for the critical mass of Wilson fermions reads

$$m_c(g^2) = g^2 m_c^{(1)} + g^4 m_c^{(2)} + \dots \quad (61)$$

Here we may use to leading order

$$Z_{\pm}^{\text{GN}}(g^2 m_c^{(1)}, 0) = [\tilde{Z}(0; z_{\pm})]^N \left\{ 1 + g^2 m_c^{(1)} N V \tilde{K}(0; z_{\pm}) \right\}. \quad (62)$$

With χ vanishing at tree level we now derive (up to $O(g^4)$)

$$\chi = \frac{V g^2}{2} [\tilde{K}(0; z_-) - \tilde{K}(0; z_+)] \left\{ (N-1) [\tilde{K}(0; z_-) + \tilde{K}(0; z_+)] + 2m_c^{(1)} \right\}. \quad (63)$$

The condition that χ vanishes as a chiral order parameter fixes the one loop mass renormalization to

$$m_c^{(1)} = -\frac{N-1}{2} [\tilde{K}(0; z_-) + \tilde{K}(0; z_+)]. \quad (64)$$

Using the definitions this may also be written as

$$m_c^{(1)} = -\frac{N-1}{2} \frac{\sum_{\varepsilon \neq (0, 0)} Z(0; \varepsilon) \text{tr} G(0; 0; \varepsilon)}{\sum_{\varepsilon \neq (0, 0)} Z(0; \varepsilon)} \quad (65)$$

and the numerical value is

$$m_c^{(1)} = -(N-1) 0.3849001795 - \frac{0.2439}{L^4} + O(L^{-6}). \quad (66)$$

A.2 Two-point correlator

For the correlator (24) (for one flavor $a = b$) the following simple result is obtained

$$\langle \xi(x) \bar{\xi}(0) \rangle_z = \frac{Z_z^{\text{GN}}}{Z_+^{\text{GN}}} \left\{ 1 + g^2(N-1) \tilde{K}(m; z) \frac{\partial}{\partial m} \right\} \tilde{G}(x; m; z) + \mathcal{O}(g^4). \quad (67)$$

In this formula the partition function ratio can also be expanded and contributes in general another $\mathcal{O}(g^2)$ term. At the chiral point however it is unity for $z = z_-$ and trivially so for z_+ . The correlations defined in this paper now read

$$k_V(x_0) = \left\{ 1 + g^2(N-1) \tilde{K}(m; z_+) \frac{\partial}{\partial m} \right\} k_V^{(0)}(x_0) + \mathcal{O}(g^4) \quad (68)$$

and

$$k_S(x_0) = \frac{1}{2} \sum_{\tau=+,-} e^{N\chi\delta_{\tau,-}} \left\{ 1 + g^2(N-1) \tilde{K}(m; z_\tau) \frac{\partial}{\partial m} \right\} k_S^{(0,\tau)}(x_0) + \mathcal{O}(g^4). \quad (69)$$

Using results from appendix A in [7] we find (for $0 < x_0 < L_0$)

$$\begin{aligned} k_V^{(0)}(x_0) = & \frac{1}{(1+m)\tilde{Z}(m; z_+)} \times \left\{ Z(m, (1, 0)) \frac{\cosh[\omega(L_0/2 - x_0)]}{\cosh[\omega L_0/2]} \right. \\ & \left. - Z(m, (0, 0)) \frac{\sinh[\omega(L_0/2 - x_0)]}{\sinh[\omega L_0/2]} \right\} \end{aligned} \quad (70)$$

where $\omega = \ln(1+m)$ is the pole mass. For small m we obtain

$$(1+m)k_V^{(0)}(x_0) \simeq 2c_{10}(1 - c_{00}mL_0) - 2c_{00}m(L_0 - 2x_0) + \mathcal{O}(m^2) \quad (71)$$

with another constant

$$c_{10} = \frac{Z(0; (1, 0))}{\sum_{\varepsilon \neq (0,0)} Z(0; \varepsilon)} = 0.313557560 - \frac{0.2199}{L^2} + \mathcal{O}(L^{-4}). \quad (72)$$

For the scalar correlator we derive

$$\begin{aligned} k_S^{(0,\pm)}(x_0) = & \frac{1}{(1+m)\tilde{Z}(m; z_\pm)} \times \left\{ Z(m, (1, 0)) \frac{\sinh[\omega(L_0/2 - x_0)]}{\cosh[\omega L_0/2]} \right. \\ & \left. \mp Z(m, (0, 0)) \frac{\cosh[\omega(L_0/2 - x_0)]}{\sinh[\omega L_0/2]} \right\}. \end{aligned} \quad (73)$$

In this case we find for small m

$$(1+m)k_S^{(0,\pm)}(x_0) = 2c_{10}m(L_0/2 - x_0) \mp 4c_{00} + \mathcal{O}(m^2). \quad (74)$$

If we combine the above results we find that the alternative order parameters $\tilde{\chi}_n$ vanish also at $O(g^2)$ if we set $m = g^2 m_c^{(1)}$, i.e. the $O(a)$ contributions seen numerically start (presumably) at $O(g^4)$ only.

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